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The SW-RPA Self-Diffusion Coefficient of Liquid Potassium

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Abstract

The self-diffusion coefficient of the liquid potassium at *T*=337K is calculated in the square-well model within the random phase approximation. A good agreement with available experimental data is obtained.

Keywords: Square-well model, random phase approximation, self-diffusion coefficient, liquid metal

In our previous works [1, 2] the square-well (SW) model within the random phase approximation with the hard-sphere reference system had been successfully applied to study the structure factor, $S(q)$, and the self-diffusion coefficient, $D=(\beta\xi)^{-1}$ (where ξ is the friction coefficient, $\beta=(k_{\mathrm{B}}T)^{-1}$, k_{B} - Boltzmann constant, T - temperature), of liquid Na near the melting point. Here, this approach is used to calculate D of the liquid K at the same condition.

The Davis-Palyvos [3] approach is used for this aim:

$$\xi=\xi_{\mathrm{H}}+\xi_{\mathrm{S}}+\xi_{\mathrm{SH}} \quad , \tag{1}$$

where ξ_{H} and ξ_{S} are the contributions due to the hard and soft part of the pair interaction, respectively, ξ_{SH} - the cross-correlation term:

$$\xi_{\mathrm{H}}=\frac{8}{3}\rho\sigma^2 g(\sigma)(\pi M/\beta)^{1/2} \quad , \tag{2}$$

$$\xi_{\mathrm{S}}=-\frac{(\beta\pi M)^{1/2}}{12\pi^2}\int_0^\infty [S(q)-1]\phi(q)q^3\mathrm{d}q \quad , \tag{3}$$

$$\xi_{\mathrm{SH}}=-\frac{1}{3}\rho\, g(\sigma)(\beta M/\pi)^{1/2}\int_0^\infty [q\sigma\cos(q\sigma)-\sin(q\sigma)]\phi(q)\mathrm{d}q \quad , \tag{4}$$

where ρ is the mean atomic density (taken here from [4]), σ - hard-core diameter, $g(r)$ - radial distribution function, M - atomic mass, $\phi(q)$ - Fourier transform of the soft part of the pair potential. The SW model parameters for liquid K are defined by fitting the first peak of $S(q)$ with respect to the experimental one [5].

Calculated D is compared with two experimental results (Table 1). Like the case of liquid Na [2], it can be seen that the SW model gives slightly overstated value of D in comparison with experimental ones.

Table 1. Self-diffusion coefficient of liquid K at T = 337 K.

	SW	Experiment [6]	Experiment [7]
$D \cdot 10^{-9}$ (m^2/s)	4.54	3.76	3.59

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